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The flexibility of Daubechies wavelets for Linear Scaling DFT calculations LUIGI GENOVESE, STEPHAN MOHR, Commissariat l'nergie Atomique et aux nergies Alternatives, LAURA ELISABETH RATCLIFF, Argonne National Laboratory, DAMIEN CALISTE, THIERRY DEUTSCH, Commissariat l'nergie Atomique et aux nergies Alternatives, STEFAN GOEDECKER, Basel University — In recent works, we presented the linear scaling version of the BigDFT code [1] based on Daubechies wavelets, where a minimal set of localized support functions is optimized in situ. Our linear scaling approach is able to generate support functions for systems in various boundary conditions, like isolated, surface and periodic [2], and it is based on a algorithm which is universally applicable, requiring only moderate amount of computing resources. We will present how the flexibility of this approach is helpful in providing a basis set that is optimally tuned to the chemical environment surrounding each atom. In addition than providing a basis useful to project Kohn-Sham orbitals informations like atomic charges and partial density of states, it can also be reused as-is, i.e. without reoptimization, for charge-constrained DFT calculations within a fragment approach [3]. We demonstrate the interest of this approach to express highly precise and efficient calculations for preparing diabatic states and for the computational setup of systems in complex environments [4]. [1] J. Chem. Phys. 140, 204110 (2014) [2] Phys. Chem. Chem. Phys., 2015, DOI: 10.1039/C5C P00437C [3] J. Chem. Phys. 142, 23, 234105 (2015) [4] J.Chem. Theory Comput. 2015, 11, 2077

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